UNIVERSITY OF TORONTO

Differential Equations of Mathematical Physics
(APM 351 Y)

2013–2014
Problem Sheet 17
(2014.02.27)

Quantum Mechanics

Homework Problems

54. The energy functional for the quantum harmonic oscillator

Define the average energy

$$\mathbb{E}_\varphi(H) := \int_{\mathbb{R}} \mathrm{d}x \, \left(\frac{1}{2m} \bigl|\varphi'(x)\bigr|^2 + V(x) \, \bigl|\varphi(x)\bigr|^2 \right) =: \mathbb{E}_\varphi\bigl(-\tfrac{1}{2m}\partial_x^2\bigr) + \mathbb{E}_\varphi(V)$$

associated to the hamiltonian $H = -\frac{1}{2m}\partial_x^2 + V$ and $\psi \in \mathcal{S}(\mathbb{R})$, seen as the sum of kinetic energy $\mathbb{E}_\varphi\bigl(-\frac{1}{2m}\partial_x^2\bigr)$ and potential energy $\mathbb{E}_\varphi(V)$.

Consider the case of the harmonic oscillator where $V(x) = \frac{m}{2}\omega^2 x^2$ is the potential energy and $\omega > 0$ the characteristic frequency of the oscillator. Moreover, define the family of scaled Gaußians $\varphi_\lambda(x) := \pi^{-1/4} \sqrt{\lambda} \, \mathrm{e}^{-\frac{\lambda^2}{2} x^2}$, $\lambda > 0$.

(i) Determine the expected value of the energy $E(\lambda) := \mathbb{E}_{\varphi_\lambda}(H)$ as a function of λ.

(ii) Find the λ_{min} which minimizes $E(\lambda)$. Give the minimizing wavefunction $\varphi_0 := \varphi_{\lambda_{\mathrm{min}}}$.

(iii) For which λ is the expected value of the kinetic energy small? What about the potential energy? Interpret your results.

(iv) Determine $E_0 \in \mathbb{R}$ so that φ_0 from (ii) satisfies the eigenvalue equation

$$H\varphi_0 = E_0 \, \varphi_0 .$$

55. The free relativistic Schrödinger operator

Consider the free relativistic Schrödinger operator $H := \sqrt{m^2 - \Delta_x}$ on $L^2(\mathbb{R}^d)$ defined as in problem 4 of Test 2.

(i) Compute $\sigma(H)$.

(ii) Determine the nature of the spectrum, i. e. determine $\sigma_{\mathrm{ess}}(P)$, $\sigma_{\mathrm{disc}}(P)$, $\sigma_{\mathrm{cont}}(P)$ and $\sigma_{\mathrm{p}}(P)$.

(iii) Are the eigenfunctions elements of the Hilbert space?

56. The Wigner transform: fundamental properties

The Wigner transform of a Schwartz function $\psi \in \mathcal{S}(\mathbb{R})$ is defined as

$$\bigl(\mathcal{W}(\psi)\bigr)(x,\xi) := \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i} y \xi} \, \overline{\psi\bigl(x - \tfrac{\varepsilon}{2} y\bigr)} \, \psi\bigl(x + \tfrac{\varepsilon}{2} y\bigr)$$

where x is position and ξ is momentum.

(i) Show that $\mathcal{W}(\psi)$ is a real-valued function on phase space $\mathbb{R}^2$.

(ii) Compute the marginals of the Wigner transform,

$$\int_{\mathbb{R}} \mathrm{d}x \, \bigl(\mathcal{W}(\psi)\bigr)(x,\xi), \qquad \int_{\mathbb{R}} \mathrm{d}\xi \, \bigl(\mathcal{W}(\psi)\bigr)(x,\xi), \qquad \int_{\mathbb{R}^2} \mathrm{d}x \, \mathrm{d}\xi \, \bigl(\mathcal{W}(\psi)\bigr)(x,\xi).$$

(iii) Show $\bigl(\mathcal{W}(T_{x'}\psi)\bigr)(x,\xi) = \bigl(\mathcal{W}(\psi)\bigr)(x - x', \xi)$ where $(T_{x'}\psi)(x) := \psi(x - x')$.

57. The Wigner transform: computations of Wigner transforms

Define the Wigner transform as in problem 56 but set $\varepsilon = 1$.

(i) Compute the Wigner transform of $\psi(x) = \mathrm{e}^{+\mathrm{i}\xi_c \, x} \, \mathrm{e}^{-\frac{x^2}{2b^2}}$. Explain at what point in $\mathbb{R}^2$ the Wigner transformed function takes its maximum.

(ii) Which roles do the parameters b and ξ_c from part (i) play? What does the Wigner transform of $\psi(x - x_c)$ look like?

(iii) Compute the Wigner transform of $\varphi(x) = x \, \mathrm{e}^{-\frac{x^2}{4}}$.

(iv) Can the Wigner transform be interpreted as a classical state?

58. Ground state of the cut off Lenard-Jones potential

Consider the hamiltonian $H_\lambda = -\partial_x^2 + \lambda V$, $\lambda > 0$, for the cut off Lenard-Jones potential

$$V(x) = \begin{cases} \frac{1}{|x|^{12}} - \frac{1}{|x|^6} & |x| \geq 1 \\ 0 & |x| < 1 \end{cases}$$

in one dimension.

(i) Show that there exists a $\lambda_0 > 0$ such that for all $0 < \lambda < \lambda_0$ the hamiltonian H_λ has a unique bound state of energy $E_\lambda < 0$.

(ii) Compute E_λ to leading order in λ.

Hand in home work on: Thursday, 6 March 2014, before class